

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.85            | 1.14 | 0.85           | 1.12 | 0.83       | 1.23 |

## Model Results

**Predicted value:**  $2.36 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.78 \times 10^{-1}$

**Confidence level:**  $7.16 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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EPTC

**Measured:**  $3.18 \times 10^{-11}$

**Predicted:**  $2.83 \times 10^{-11}$

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Cycloate

**Measured:**  $3.54 \times 10^{-11}$

**Predicted:**  $2.98 \times 10^{-11}$

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p-Nitroanisole

**Measured:**  $2.46 \times 10^{-12}$

**Predicted:**  $1.65 \times 10^{-11}$

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Triethyl phosphate

**Measured:**  $5.53 \times 10^{-11}$

**Predicted:**  $4.26 \times 10^{-11}$

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1-Nitro-2-methylnaphthalene

**Measured:**  $8.00 \times 10^{-12}$

**Predicted:**  $3.49 \times 10^{-11}$